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The Main Characteristics of the Wills-Harrison Effective Pair Potential in Liquid Co

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Abstract

It is found that the position of the first minimum of the Wills-Harrison effective pair potential in liquid Co begins to shift significantly to the right-hand side when the *d*-*d*-non-diagonal coupling begins to predominate in the metal under consideration.

Keywords: Transition metal, Wills-Harrison pair potential, *d*-state coupling

In [1] the Wills-Harrison (WH) model [2] was corrected by means the introduction the probability p that all 25 *d*-*d* couplings between two different atoms are equiprobable and probability $(1-p)$ that only 5 equiprobable diagonal couplings are possible.

Here, we consider how the magnitude p influences the position, $r_{\min}$, and the magnitude of the first minimum of the WH effective pair potential, $\varphi_{\mathrm{WH}}(r)$, in liquid Co. Earlier, the analogous study was fulfilled for liquid Fe [3].

We use the local Bretonnet-Silbert (BS) model pseudopotential [4] for description the *s*-electron contribution to $\varphi_{\mathrm{WH}}(r)$. Input data (WH and BS parameters and the experimental mean atomic volume, Ω) are listed in Table 1.

It is found that behaviors of both curves (Figs. 1- 2) are similar that in liquid Fe [3]: the magnitude of the first minimum quite monotonously increases with increasing p, but the first-minimum position begins to increase harshly from $p = 0.6$ approximately. It denotes that significant shift of the $\varphi_{\mathrm{WH}}(r)$ first minimum to the right-hand side is occurred in liquid Co when the non-diagonal coupling begins to predominate. The same tendency was found in liquid Fe [3].

Table 1. Input data for calculation

r_d (a.u.) [2]	z_s [5]	z_d [5]	R_C (a.u.) [5]	a (a.u.) [5]	Ω (a.u.) [6]
1.437	1.4	7.6	1.64	0.393	85.85

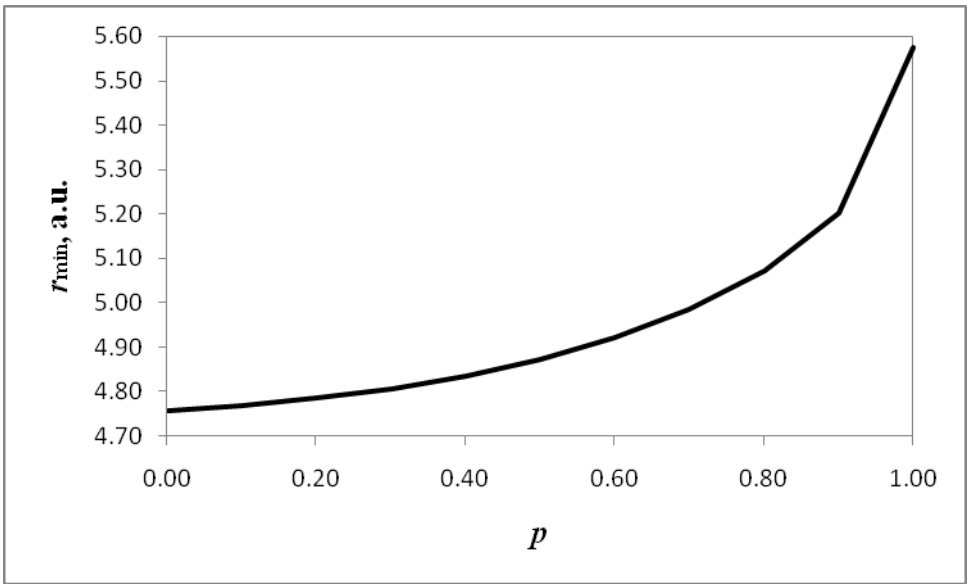

Figure 1. $r_{\min}$ of $\varphi_{WH}(r)$ in liquid Co at different p (T=1863K).

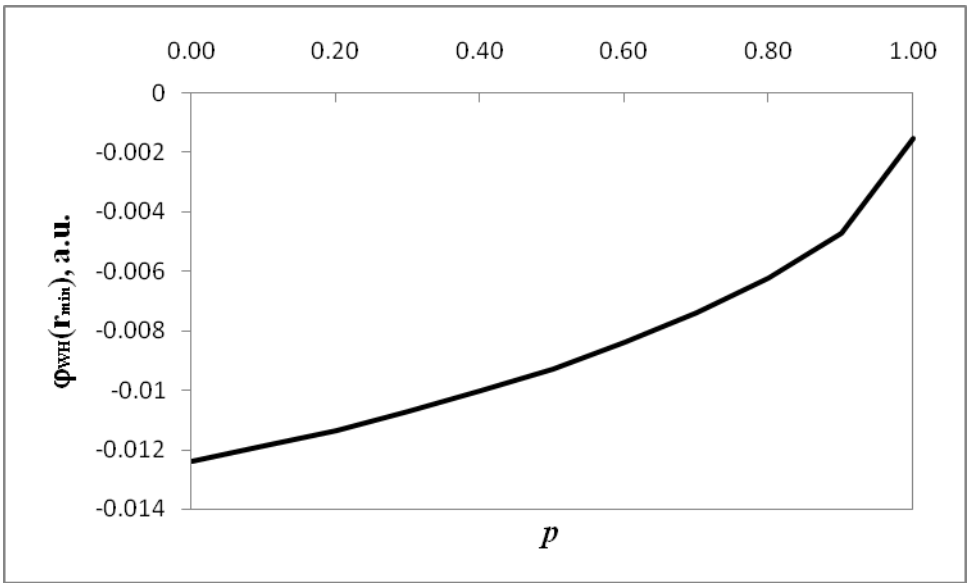

Figure 2. $\varphi_{WH}(r_{\min})$ in liquid Co at different p (T=1863K).

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